



# **STIC Search Report**

## **EIC 1700**

**STIC Database Tracking Number: 122138**

**TO: Ben Sackey**  
**Location: REM 5B31**  
**Art Unit : 1626**  
**May 19, 2004**

**Case Serial Number: 10/088276**

**From: Kathleen Fuller**  
**Location: EIC 1700**  
**REMSSEN 4B28**  
**Phone: 571/272-2505**  
**Kathleen.Fuller@uspto.gov**

### **Search Notes**

Ms Fuller

Access DB# 122138

## SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: BEN SACKLEY Examiner #: 73489 Date: 5/15/04  
Art Unit: 1626 Phone Number 302-0704 Serial Number: 101088, 276  
Mail Box and Bldg/Room Location: Rem 5831 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

\*\*\*\*\*

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Process for preparing fused pyrazoles

Inventors (please provide full names): Makoto Tokunaga et al.

Earliest Priority Filing Date: 7/17/200

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

process for preparing condensed pyrazoles comprising reacting:  
alkyne alcohol of formula (4)  
$$\text{HC}\equiv\text{C}-\text{C}(\text{R}^1)(\text{R}^2)-\text{R}^3$$
 with aromatic primary amine in the presence of Ruthenium complex

\*\*\*\*\*

### STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: <u>X. Fuller</u>	NA Sequence (#) _____	STN <u>✓</u>
Searcher Phone #: _____	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) <u>4</u>	Questel/Orbit _____
Date Searcher Picked Up: _____	Bibliographic _____	Dr.Link _____
Date Completed: <u>5/19/04</u>	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: <u>20</u>	Fulltext _____	Sequence Systems _____
Clerical Prep Time: _____	Patent Family _____	WWW/Internet _____
Online Time: <u>50</u>	Other _____	Other (specify) _____

PTO-1590 (8-01)

Casread prep

=> FILE CASREAC

FILE 'CASREACT' ENTERED AT 15:21:45 ON 19 MAY 2004  
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FILE CONTENT:1840 - 16 May 2004 VOL 140 ISS 20

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

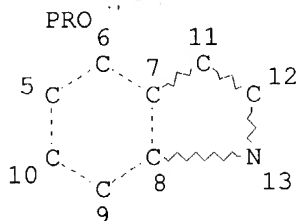
Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> D QUE L7

L3 STR

RRT

CH≡C~C~OH  
1 2 3 4



NODE ATTRIBUTES:

NSPEC IS RC AT 3  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L5 54 SEA FILE=CASREACT SSS FUL L3 ( 334 REACTIONS)  
L6 33 SEA FILE=CASREACT ABB=ON L5(L)ANY/CAT  
L7 3 SEA FILE=CASREACT ABB=ON L6 AND (RU OR RUTHENIUM).

=> D L7 1-3 BIB ABS FHIT

L7 ANSWER 1 OF 3 CASREACT COPYRIGHT 2004 ACS on STN

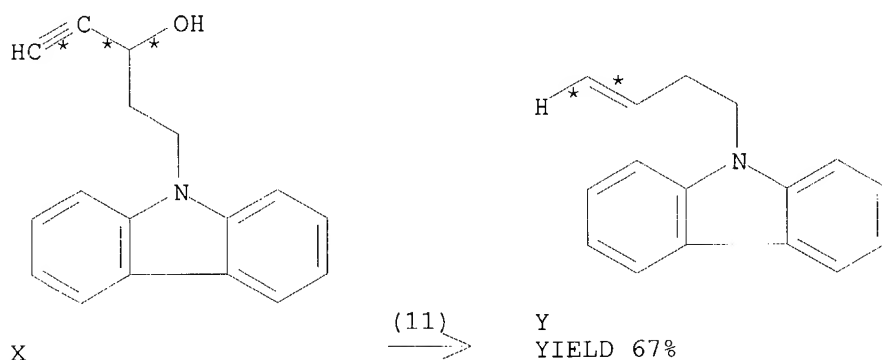
AN 139:230387 CASREACT

TI A New **Ruthenium**-Catalyzed Cleavage of a Carbon-Carbon Triple  
Bond: Efficient Transformation of Ethynyl Alcohol into Alkene and Carbon  
Monoxide

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

AU Datta, Swarup; Chang, Chia-Lung; Yeh, Kuo-Liang; Liu, Rai-Shung  
 CS Department of Chemistry, National Tsing-Hua University, Hsinchu, Taiwan,  
 30043, Peop. Rep. China  
 SO Journal of the American Chemical Society (2003), 125(31), 9294-9295  
 CODEN: JACSAT; ISSN: 0002-7863  
 PB American Chemical Society  
 DT Journal  
 LA English  
 AB A new and efficient **ruthenium**-catalyzed reaction that transforms  
 ethynyl alc. into alkene and carbon monoxide is reported. The most  
 efficient catalysts are  $\text{TpRu}(\text{PPh}_3)(\text{MeCN})_2\text{PF}_6$  (10 mol %) and lithium  
 triflate (20 mol %). The mechanism of this reaction was elucidated using  
 an isotope-labeling experiment

RX(11) OF 18 X ==> Y

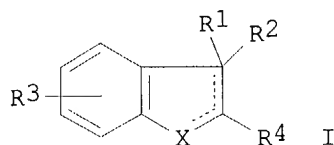


RX(11) RCT X 591760-14-4  
 PRO Y 10420-18-5  
 CAT 443306-65-8 Ruthenium(1+),  
 bis(acetonitrile)[hydrotris(1H-pyrazolato- $\kappa\text{N1}$ )borato(1-)-  
 $\kappa\text{N2}, \kappa\text{N2}', \kappa\text{N2}''$ ](triphenylphosphine)-,  
 (OC-6-23)-, hexafluorophosphate(1-), 33454-82-9  
 CF3SO3Li  
 SOL 108-88-3 PhMe  
 NTE stereoselective  
 RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 3 CASREACT COPYRIGHT 2004 ACS on STN  
 AN 136:118383 CASREACT  
 TI Processes for preparation of indole derivatives  
 IN Tokunaga, Makoto; Wakatsuki, Yasuo  
 PA Japan Science and Technology Corporation, Japan; Riken Corp.  
 SO PCT Int. Appl., 27 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

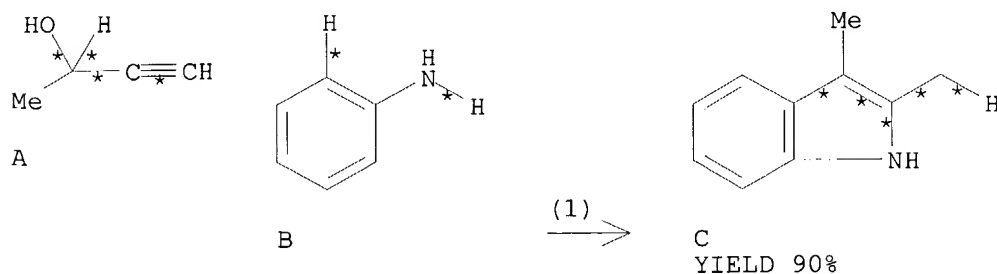
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002006226	A1	20020124	WO 2001-JP5691	20010702

W: US  
 RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,  
 PT, SE, TR  
 JP 2002030069 A2 20020129 JP 2000-216457 20000717  
 EP 1302459 A1 20030416 EP 2001-945742 20010702  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, FI, CY, TR  
 US 2004049054 A1 20040311 US 2002-88276 20021022  
 PRAI JP 2000-216457 20000717  
 WO 2001-JP5691 20010702  
 OS MARPAT 136:118383  
 GI



AB The invention provides processes for the preparation of fused pyrroles, preferably indoles, which permit the use of inexpensive aromatic amines themselves as the raw material and attain high atomic efficiency and high regioselectivity. Specifically, a process for the preparation of fused pyrroles, e.g., indoles [I; R1 = CH3, H, C6H5, CH3CH2, CH3(CH2)2; R2 = H, CH3, alkyl, aryl, electron pair; R1R2 = alkylene; R3 = H, 3-HO, 4-CH3O, 3,4-(CH3O)2, 4-CH3, 2-CH3, 4-Cl, 2-CH3OCO; R4 = H, CH3, C6H5, CH3CH2, CH3(CH2)2; X = N, NH; dotted bond = single, double] characterized by reacting an alkynol, HCCCHR1OH with an aromatic primary amine, R3C6H4NH2 in the presence of a **ruthenium** complex (Ru3(CO)12), more preferably with an acid or an ammonium salt (NH4·PF6). Thus, the title compound I (R1 = H; R2 = electron pair; R3 = H; R4 = (CH2)4CH3; X = NH; single bond at XCH; double at CH:CH) was prepared from CH3(CH2)4CHOHCCCH and C6H5NH2 in the presence of Ru3(CO)12.

RX(1) OF 13      A + B ==> C

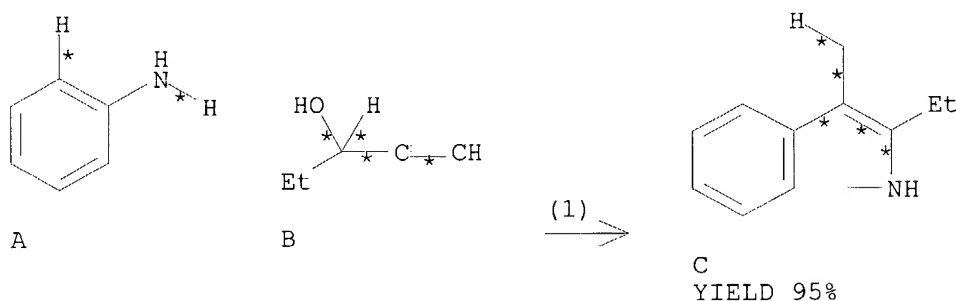


RX(1)      RCT    A **2028-63-9**, B 62-53-3  
 RGT    D 142-04-1 PhNH2.HCl  
 PRO    C **91-55-4**  
 CAT    **15243-33-1** Ru3(CO)12  
 NTE    120°, 12 h, regioselective  
 RE.CNT    6      THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD

## ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 3 CASREACT COPYRIGHT 2004 ACS on STN  
AN 135:166752 CASREACT  
TI A practical one-pot synthesis of 2,3-disubstituted indoles from unactivated anilines  
AU Tokunaga, M.; Ota, M.; Haga, M.-a.; Wakatsuki, Y.  
CS PRESTO, Japan Science and Technology Corporation (JST), Saitama, 332-0012, Japan  
SO Tetrahedron Letters (2001), 42(23), 3865-3868  
CODEN: TELEAY; ISSN: 0040-4039  
PB Elsevier Science Ltd.  
DT Journal  
LA English  
AB 2-Substituted 3-methylindoles are synthesized with good regioselectivity from readily available substrates and catalysts, i.e., the reaction of anilines with propargyl alcs. in the presence of 0.36-1 mol % Ru<sub>3</sub>(CO)<sub>12</sub>.

RX(1) OF 10 A + B ==&gt; C



RX(1) RCT A 62-53-3, B 4187-86-4  
PRO C 19013-49-1  
CAT 15243-33-1 Ru<sub>3</sub>(CO)<sub>12</sub>, 142-04-1 PhNH<sub>2</sub>.HCl  
NTE regioselective, no solvent, reaction run in open air, optimization study, optimized on catalyst  
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; =&gt; FILE REG

FILE 'REGISTRY' ENTERED AT 15:42:06 ON 19 MAY 2004  
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Property values tagged with IC are from the ZIC/VINITI data file  
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STRUCTURE FILE UPDATES: 18 MAY 2004 HIGHEST RN 683203-75-0  
DICTIONARY FILE UPDATES: 18 MAY 2004 HIGHEST RN 683203-75-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> FILE HCAPLUS

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FILE COVERS 1907 - 19 May 2004 VOL 140 ISS 21

FILE LAST UPDATED: 18 May 2004 (20040518/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> D QUE

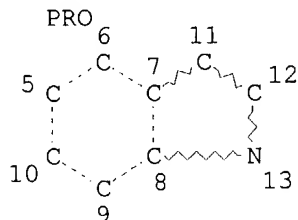
L2 34 SEA FILE=REGISTRY ABB=ON (10257-92-8/BI OR 104-94-9/BI OR 105-31-7/BI OR 105908-32-5/BI OR 106-47-8/BI OR 106-49-0/BI OR 107-21-1/BI OR 13141-50-9/BI OR 134-20-3/BI OR 134-32-7/BI OR 142-04-1/BI OR 15243-33-1/BI OR 16941-11-0/BI OR 19013-49-1/BI OR 2028-63-9/BI OR 21296-93-5/BI OR 27505-78-8/BI OR 36729-21-2/BI OR 36729-23-4/BI OR 391611-81-7/BI OR 391611-82-8/BI OR 4187-86-4/BI OR 4187-87-5/BI OR 4757-69-1/BI OR 591-27-5/BI OR 62-53-3/BI OR 6315-89-5/BI OR 73177-34-1/BI OR 78-27-3/BI OR 818-72-4/BI OR 828-94-4/BI OR 89188-94-3/BI OR 91-55-4/BI OR 95-53-4/BI)

L3

STR

RRT

CH=C~C~OH  
 1 2 3 4



NODE ATTRIBUTES:

NSPEC IS RC AT 3

DEFAULT MLEVEL IS ATOM

KATHLEEN FULLER EIC 1700 REMSEN 4B28 571/272-2505

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L5 54 SEA FILE=CASREACT SSS FUL L3 ( 334 REACTIONS)  
L6 33 SEA FILE=CASREACT ABB=ON L5(L)ANY/CAT  
L7 3 SEA FILE=CASREACT ABB=ON L6 AND (RU OR RUTHENIUM)  
L17 564549 SEA FILE=REGISTRY ABB=ON 333.151/RID  
L18 564549 SEA FILE=REGISTRY ABB=ON L17 OR L17  
L19 294550 SEA FILE=REGISTRY RAN=(,231942-50-0) ABB=ON L17 OR L17  
L20 269999 SEA FILE=REGISTRY ABB=ON L18 NOT L19  
L21 262767 SEA FILE=HCAPLUS ABB=ON L19  
L22 21622 SEA FILE=HCAPLUS ABB=ON L20  
L23 47043 SEA FILE=HCAPLUS ABB=ON (L21 OR L22) (L) (PREP OR IMF OR  
SPN)/RL  
L24 7 SEA FILE=HCAPLUS ABB=ON L23 AND (ALKYNOL# OR ALKYNE ALC?)  
L25 75 SEA FILE=HCAPLUS ABB=ON L23 AND (RU OR RUTHENIUM) (L) CAT/RL  
L26 5 SEA FILE=HCAPLUS ABB=ON L25 AND ALKYN?  
L27 11 SEA FILE=REGISTRY ABB=ON L2 AND OL  
L28 5 SEA FILE=REGISTRY ABB=ON L27 AND YNYL  
L29 2077 SEA FILE=HCAPLUS ABB=ON L28  
L30 40 SEA FILE=HCAPLUS ABB=ON L23 AND L29  
L31 2 SEA FILE=HCAPLUS ABB=ON L25 AND L30  
L33 5 SEA FILE=HCAPLUS ABB=ON (L24 OR L26) AND (RU OR RUTHEN?) (L) CAT  
/RL  
L34 6 SEA FILE=HCAPLUS ABB=ON L31 OR L33  
L35 3 SEA FILE=HCAPLUS ABB=ON L7  
L36 6 SEA FILE=HCAPLUS ABB=ON (L34 OR L35) NOT L35

=> D L35 ALL 1-6 HITSTR

L35 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 2003:519850 HCAPLUS  
DN **139:230387**  
ED Entered STN: 09 Jul 2003  
TI A New Ruthenium-Catalyzed Cleavage of a Carbon-Carbon Triple Bond:  
Efficient Transformation of Ethynyl Alcohol into Alkene and Carbon  
Monoxide  
AU Datta, Swarup; Chang, Chia-Lung; Yeh, Kuo-Liang; Liu, Rai-Shung  
CS Department of Chemistry, National Tsing-Hua University, Hsinchu, Taiwan,  
30043, Peop. Rep. China  
SO Journal of the American Chemical Society (2003), 125(31), 9294-9295  
CODEN: JACSAT; ISSN: 0002-7863  
PB American Chemical Society  
DT Journal  
LA English  
CC 25-2 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
OS CASREACT 139:230387  
AB A new and efficient ruthenium-catalyzed reaction that transforms ethynyl  
alc. into alkene and carbon monoxide is reported. The most efficient  
catalysts are TpRu(PPh3)(MeCN)2PF6 (10 mol %) and lithium triflate (20 mol  
%). The mechanism of this reaction was elucidated using an  
isotope-labeling experiment  
ST ethynyl alc cleavage alkene carbon monoxide ruthenium catalyst  
IT Alcohols, reactions



RL: RCT (Reactant); RACT (Reactant or reagent)  
(acetylenic; transformation of ethynyl alcs. into alkenes and carbon  
monoxide by ruthenium-catalyzed cleavage of the triple bond)

IT Elimination reaction  
Elimination reaction catalysts  
(transformation of ethynyl alcs. into alkenes and carbon monoxide by  
ruthenium-catalyzed cleavage of the triple bond)

IT Alkenes, preparation  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(transformation of ethynyl alcs. into alkenes and carbon monoxide by  
ruthenium-catalyzed cleavage of the triple bond)

IT 33454-82-9, Lithium triflate 443306-65-8  
RL: CAT (Catalyst use); USES (Uses)  
(transformation of ethynyl alcs. into alkenes and carbon monoxide by  
ruthenium-catalyzed cleavage of the triple bond)

IT 53735-49-2, 1-Undecyn-3-ol 591760-04-2 591760-05-3 591760-06-4  
591760-07-5 591760-08-6 591760-09-7 591760-10-0 591760-11-1  
591760-12-2 591760-13-3 591760-14-4 591760-15-5 591760-16-6  
591760-17-7 591760-18-8 591760-19-9 591760-27-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(transformation of ethynyl alcs. into alkenes and carbon monoxide by  
ruthenium-catalyzed cleavage of the triple bond)

IT 94-59-7P 872-05-9P, 1-Decene 2294-81-7P 2489-88-5P 10420-18-5P  
14966-05-3P 15451-33-9P 18491-21-9P 20574-98-5P 117749-13-0P  
163268-25-5P 190334-82-8P 591760-20-2P 591760-21-3P 591760-22-4P  
591760-23-5P 591760-25-7P 591760-29-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(transformation of ethynyl alcs. into alkenes and carbon monoxide by  
ruthenium-catalyzed cleavage of the triple bond)

RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE

(1) Anon; Transition Metals in the Synthesis of Complex Organic Molecules 1994,  
P237

(2) Bianchini, C; J Am Chem Soc 1996, V118, P4585 HCAPLUS

(3) Brizius, G; Org Lett 2002, V4, P2829 HCAPLUS

(4) Bruneau, C; Acc Chem Res 1999, V32, P311 HCAPLUS

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(6) Bustelo, E; J Am Chem Soc 2003, V125, P3311 HCAPLUS

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(10) Chin, C; Organometallics 2002, V21, P1739 HCAPLUS

(11) Davies, S; Adv Organomet Chem 1990, V30, P30

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(13) Furstner, A; Angew Chem, Int Ed 1998, V37, P1734 HCAPLUS

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Organometallics in Organic Synthesis 1995, V12

(18) Jennings, P; Chem Rev 1994, V94, P2241 HCAPLUS

(19) Jun, C; J Am Chem Soc 2001, V123, P8600 HCAPLUS

(20) Knaup, W; J Organomet Chem 1991, V411, P471 HCAPLUS

(21) Lee, D; J Am Chem Soc 2003, V125

(22) Madhushaw, R; J Am Chem Soc 2001, V123, P7427 HCAPLUS

(23) McCullough, G; J Am Chem Soc 1984, V106, P4067

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P97 HCAPLUS

- (26) Nishibayashi, Y; J Am Chem Soc 2000, V122, P11019 HCAPLUS  
(27) O'Connor, J; J Am Chem Soc 1990, V112, P9013 HCAPLUS  
(28) O'Connor, J; J Chem Soc, Chem Commun 1995, P1209 HCAPLUS  
(29) Rybchinski, B; Angew Chem, Int Ed 1999, V38, P870  
(30) Sawaki, Y; Bull Chem Soc Jpn 1983, V56, P1133 HCAPLUS  
(31) Shimada, T; J Am Chem Soc 2003, V125  
(32) Trost, B; J Am Chem Soc 1992, V114, P5476 HCAPLUS  
(33) Trost, B; Tetrahedron Lett 1994, V35, P4059 HCAPLUS  
(34) Werner, H; Organometallics 1997, V16(6), P4077  
(35) Yeh, K; J Am Chem Soc 2002, V124, P6510 HCAPLUS

L35 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:72041 HCAPLUS

DN **136:118383**

ED Entered STN: 25 Jan 2002

TI Processes for preparation of indole derivatives

IN Tokunaga, Makoto; Wakatsuki, Yasuo

PA Japan Science and Technology Corporation, Japan; Riken Corp.

SO PCT Int. Appl., 27 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

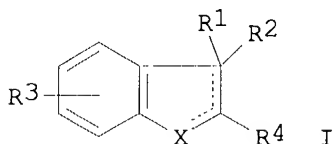
IC ICM C07D209-08

ICS C07D209-96

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	WO 2002006226	A1	20020124	WO 2001-JP5691	20010702
	W: US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
	JP 2002030069	A2	20020129	JP 2000-216457	20000717
	EP 1302459	A1	20030416	EP 2001-945742	20010702
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
	US 2004049054	A1	20040311	US 2002-88276	20021022
PRAI	JP 2000-216457	A	20000717		
	WO 2001-JP5691	W	20010702		
OS	CASREACT 136:118383; MARPAT 136:118383				
GI					



AB The invention provides processes for the preparation of fused pyrroles, preferably indoles, which permit the use of inexpensive aromatic amines themselves as the raw material and attain high atomic efficiency and high regioselectivity. Specifically, a process for the preparation of fused pyrroles, e.g., indoles [I; R1 = CH3, H, C6H5, CH3CH2, CH3(CH2)2; R2 = H, CH3, alkyl, aryl, electron pair; R1R2 = alkylene; R3 = H, 3-HO, 4-CH3O, 3,4-(CH3O)2, 4-CH3, 2-CH3, 4-Cl, 2-CH3OCO; R4 = H, CH3, C6H5, CH3CH2, CH3(CH2)2; X = N, NH; dotted bond = single, double] characterized by

reacting an alkynol, HCCCHR1OH with an aromatic primary amine, R3C6H4NH2 in the presence of a ruthenium complex (Ru3(CO)12), more preferably with an acid or an ammonium salt (NH4·PF6). Thus, the title compound I (R1 = H; R2 = electron pair; R3 = H; R4 = (CH2)4CH3; X = NH; single bond at XCH; double at CH:CH) was prepared from CH3(CH2)4CHOHCCH and C6H5NH2 in the presence of Ru3(CO)12.

ST indole prepn catalysis ruthenium carbonyl complex catalyst

IT Catalysis

Catalysts

Regiochemistry

(processes for preparation of indole derivs.)

IT 15243-33-1, Triruthenium dodecacarbonyl

RL: CAT (Catalyst use); USES (Uses)

(processes for preparation of indole derivs.)

IT 62-53-3, Aniline, reactions 78-27-3, 1-Ethynyl-1-cyclohexanol 95-53-4,

2-Methylaniline, reactions 104-94-9, 4-Methoxyaniline 105-31-7,

1-Hexyn-3-ol 106-47-8, 4-Chloroaniline, reactions 106-49-0,

4-Methylaniline, reactions 134-20-3, 2-Methoxycarbonylaniline

134-32-7, 1-Naphthylamine 142-04-1, Aniline hydrochloride 591-27-5,

3-Hydroxyaniline 818-72-4, 1-Octyn-3-ol 2028-63-9, 3-Butyn-2-ol

4187-86-4, 1-Pentyn-3-ol 4187-87-5 6315-89-5, 3,4-Dimethoxyaniline

RL: RCT (Reactant); RACT (Reactant or reagent)

(processes for preparation of indole derivs.)

IT 107-21-1, Ethylene glycol, reactions 16941-11-0, Ammonium

hexafluorophosphate

RL: RGT (Reagent); RACT (Reactant or reagent)

(processes for preparation of indole derivs.)

IT 91-55-4P, 2,3-Dimethylindole 828-94-4P 4757-69-1P 10257-92-8P

13141-50-9P 19013-49-1P 21296-93-5P 27505-78-8P 36729-21-2P

36729-23-4P 73177-34-1P 89188-94-3P 105908-32-5P 391611-81-7P

391611-82-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(processes for preparation of indole derivs.)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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L35 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:372496 HCAPLUS

DN 135:166752

ED Entered STN: 24 May 2001

TI A practical one-pot synthesis of 2,3-disubstituted indoles from unactivated anilines

AU Tokunaga, M.; Ota, M.; Haga, M.-a.; Wakatsuki, Y.

CS PRESTO, Japan Science and Technology Corporation (JST), Saitama, 332-0012, Japan

SO Tetrahedron Letters (2001), 42(23), 3865-3868

CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier Science Ltd.

DT Journal

LA English

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

OS CASREACT 135:166752

AB 2-Substituted 3-methylindoles are synthesized with good regioselectivity

from readily available substrates and catalysts, i.e., the reaction of anilines with propargyl alcs. in the presence of 0.36-1 mol % Ru<sub>3</sub>(CO)<sub>12</sub>.

ST indole disubstituted deriv one pot prepn; aniline reaction propargyl alc ruthenium carbonyl

IT Cyclization  
(practical one-pot synthesis of 2,3-disubstituted indoles from unactivated anilines)

IT Cyclization catalysts  
(triruthenium dodecacarbonyl for practical one-pot synthesis of 2,3-disubstituted indoles from unactivated anilines)

IT 15243-33-1, Triruthenium dodecacarbonyl  
RL: CAT (Catalyst use); USES (Uses)  
(practical one-pot synthesis of 2,3-disubstituted indoles from unactivated anilines)

IT 62-53-3, Aniline, reactions 95-53-4, o-Toluidine, reactions 104-94-9, p-Anisidine 106-47-8, 4-Chloroaniline, reactions 106-49-0, p-Toluidine, reactions 134-20-3, Methyl anthranilate 134-32-7, 1-Naphthylamine 142-04-1, Aniline hydrochloride 540-23-8, p-Toluidine hydrochloride 818-72-4, 1-Octyn-3-ol 2028-63-9, 3-Butyn-2-ol 4187-86-4, 1-Pentyn-3-ol 4187-87-5 16941-11-0, Ammonium hexafluorophosphate 20265-97-8, p-Anisidine hydrochloride 21436-98-6, 2,6-Dimethylaniline hydrochloride 353746-92-6 353746-93-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(practical one-pot synthesis of 2,3-disubstituted indoles from unactivated anilines)

IT 91-55-4P, 2,3-Dimethylindole 828-94-4P 10257-92-8P 19013-49-1P, 2-Ethyl-3-methylindole 21296-93-5P 27505-78-8P 36729-21-2P 73177-34-1P 89188-94-3P 105908-32-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(practical one-pot synthesis of 2,3-disubstituted indoles from unactivated anilines)

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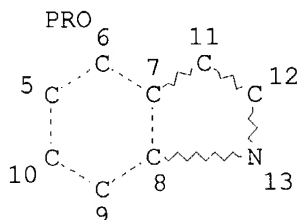
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L2 34 SEA FILE=REGISTRY ABB=ON (10257-92-8/BI OR 104-94-9/BI OR  
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 142-04-1/BI OR 15243-33-1/BI OR 16941-11-0/BI OR 19013-49-1/BI  
 OR 2028-63-9/BI OR 21296-93-5/BI OR 27505-78-8/BI OR 36729-21-2  
 /BI OR 36729-23-4/BI OR 391611-81-7/BI OR 391611-82-8/BI OR  
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 62-53-3/BI OR 6315-89-5/BI OR 73177-34-1/BI OR 78-27-3/BI OR  
 818-72-4/BI OR 828-94-4/BI OR 89188-94-3/BI OR 91-55-4/BI OR  
 95-53-4/BI)

L3 STR

RRT

CH≡C~C~C~OH  
 1 2 3 4



NODE ATTRIBUTES:

NSPEC IS RC AT 3

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L5 54 SEA FILE=CASREACT SSS FUL L3 ( 334 REACTIONS)  
 L6 33 SEA FILE=CASREACT ABB=ON L5(L)ANY/CAT  
 L7 3 SEA FILE=CASREACT ABB=ON L6 AND (RU OR RUTHENIUM)  
 L17 564549 SEA FILE=REGISTRY ABB=ON 333.151/RID  
 L18 564549 SEA FILE=REGISTRY ABB=ON L17 OR L17  
 L19 294550 SEA FILE=REGISTRY RAN=(,231942-50-0) ABB=ON L17 OR L17  
 L20 269999 SEA FILE=REGISTRY ABB=ON L18 NOT L19  
 L21 262767 SEA FILE=HCAPLUS ABB=ON L19  
 L22 21622 SEA FILE=HCAPLUS ABB=ON L20  
 L23 47043 SEA FILE=HCAPLUS ABB=ON (L21 OR L22) (L) (PREP OR IMF OR  
 SPN) /RL  
 L24 7 SEA FILE=HCAPLUS ABB=ON L23 AND (ALKYNOL# OR ALKYNE ALC?)  
 L25 75 SEA FILE=HCAPLUS ABB=ON L23 AND (RU OR RUTHENIUM) (L) CAT/RL  
 L26 5 SEA FILE=HCAPLUS ABB=ON L25 AND ALKYN?  
 L27 11 SEA FILE=REGISTRY ABB=ON L2 AND OL  
 L28 5 SEA FILE=REGISTRY ABB=ON L27 AND YNYL  
 L29 2077 SEA FILE=HCAPLUS ABB=ON L28  
 L30 40 SEA FILE=HCAPLUS ABB=ON L23 AND L29  
 L31 2 SEA FILE=HCAPLUS ABB=ON L25 AND L30  
 L33 5 SEA FILE=HCAPLUS ABB=ON (L24 OR L26) AND (RU OR RUTHEN?) (L) CAT  
 /RL  
 L34 6 SEA FILE=HCAPLUS ABB=ON L31 OR L33  
 L35 3 SEA FILE=HCAPLUS ABB=ON L7  
 L36 6 SEA FILE=HCAPLUS ABB=ON (L34 OR L35) NOT L35

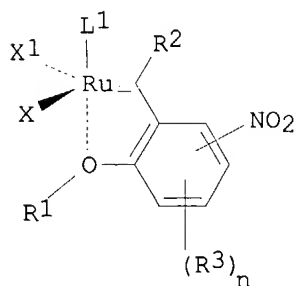
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=> D L36 ALL 1-6 HITSTR

L36 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2004:354955 HCAPLUS  
 ED Entered STN: 30 Apr 2004  
 TI Preparation of ruthenium carbene complexes as (pre)catalysts for  
 metathesis reactions  
 IN Grela, Karol  
 PA Boehringer Ingelheim International G.m.b.H., Germany  
 SO PCT Int. Appl., 30 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07F015-00  
 CC 29-13 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 21, 67

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004035596	A1	20040429	WO 2003-EP11222	20031010
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	PL 2002-356652	A	20021015		
GI					



I

AB The invention relates to the preparation of new ruthenium carbene complexes I  
 (L1 = neutral ligand; X, X1 = anionic ligands; R1 = C1-5 alkyl, C5-6

cycloalkyl; R2 = H, C1-20 alkyl, C2-20 alkenyl, C2-20 **alkynyl**, aryl; R3 = C1-6 alkyl, C1-6 alkoxy, C1-6 alkyl or alkoxy substituted aryl; n = 0-3). I are convenient (pre)catalysts for metathesis reactions and can be applied i.e. for ring-closing metathesis, cross metathesis or ene-yne metathesis reactions. Thus, CuCl-mediated reaction of 2-isopropoxy-5-nitrostyrene (preparation given) with Cl<sub>2</sub>Ru(L1)(PCy<sub>3</sub>)(:CH<sub>2</sub>Ph) (L1 = 1,3-bis(mesityl)imidazolidene) in CH<sub>2</sub>Cl<sub>2</sub> gave 83% of title I (L1 = same, X, X1 = Cl, R1 = iPr, R2, (R3)n = H, and 4-substituted NO<sub>2</sub>), which was used as cross metathesis catalyst (example given).

ST ruthenium carbene complex prepn pre catalyst ring closing metathesis;  
cross metathesis catalyst ruthenium carbene complex prepn

IT Metathesis catalysts  
(cross metathesis; preparation of ruthenium carbene complexes as catalysts for metathesis reactions)

IT Carbene complexes  
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)  
(preparation of **ruthenium** carbene complexes as catalysts for metathesis reactions)

IT Metathesis catalysts  
(ring-closing; preparation of ruthenium carbene complexes as catalysts for metathesis reactions)

IT 502964-52-5P 625082-83-9P 682349-81-1P  
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)  
(preparation of **ruthenium** carbene complexes as catalysts for metathesis reactions)

IT 75-30-9, 2-Iodopropane 96-33-3, Methyl acrylate 97-51-8 107-13-1, Acrylonitrile 1779-49-3, Methyltriphenylphosphonium bromide 2049-80-1 5309-50-2 85807-84-7 103851-61-2 104144-06-1 172222-30-9 245679-18-9 246047-72-3 606140-56-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of ruthenium carbene complexes as catalysts for metathesis reactions)

IT 166263-27-0P 173035-11-5P 502848-71-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of ruthenium carbene complexes as catalysts for metathesis reactions)

IT 2698-64-8P 57502-57-5P 125878-07-1P 340810-54-0P  
**682349-82-2P**  
RL: **SPN (Synthetic preparation); PREP (Preparation)**  
(preparation of ruthenium carbene complexes as catalysts for metathesis reactions)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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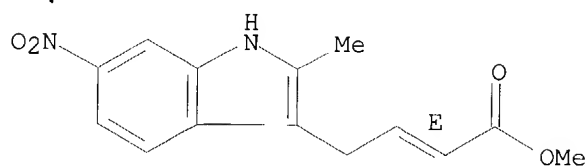
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IT **682349-82-2P**  
RL: **SPN (Synthetic preparation); PREP (Preparation)**  
(preparation of ruthenium carbene complexes as catalysts for metathesis reactions)

RN 682349-82-2 HCAPLUS

CN 2-Butenoic acid, 4-(2-methyl-6-nitro-1H-indol-3-yl)-, methyl ester, (2E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



L36 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 2003:513756 HCAPLUS  
DN 139:230569  
ED Entered STN: 06 Jul 2003  
TI Novel ruthenium- and platinum-catalyzed sequential reactions: Synthesis of tri- and tetrasubstituted furans and pyrroles from propargylic alcohols and ketones  
AU Nishibayashi, Yoshiaki; Yoshikawa, Masato; Inada, Youichi; Milton, Marilyn Daisy; Hidai, Masanobu; Uemura, Sakae  
CS Department of Energy and Hydrocarbon Chemistry Graduate School of Engineering, Kyoto University, Kyoto, 606-8501, Japan  
SO Angewandte Chemie, International Edition (2003), 42(23), 2681-2684  
CODEN: ACIEF5; ISSN: 1433-7851  
PB Wiley-VCH Verlag GmbH & Co. KGaA  
DT Journal  
LA English  
CC 27-13 (Heterocyclic Compounds (One Hetero Atom))  
OS CASREACT 139:230569  
AB The two catalysts [Cp\*RuCl( $\mu$ -2-SMe)<sub>2</sub>RuCp\*Cl] (1) and PtCl<sub>2</sub> (2) promote a sequence of catalytic cycles in the same medium. Tri- or tetrasubstituted furans or pyrroles are afforded in moderate to good yields with high regioselectivities from the catalyzed reactions of propargylic alcs. with ketones or with ketones and anilines, resp.  
ST furan prepn propargylic alc ketone platinum ruthenium catalyzed cycloaddn; pyrrole prepn propargylic alc ketone platinum ruthenium catalyzed cycloaddn  
IT Cycloaddition reaction catalysts  
(preparation of tri- and tetrasubstituted furans and pyrroles from ruthenium- and platinum- catalyzed propargylic alcs. and ketones)  
IT Ketones, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of tri- and tetrasubstituted furans and pyrroles from ruthenium- and platinum- catalyzed propargylic alcs. and ketones)  
IT Alcohols, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(propargyl; preparation of tri- and tetrasubstituted furans and pyrroles from ruthenium- and platinum- catalyzed propargylic alcs. and ketones)  
IT 10025-65-7, Platinum dichloride 216064-20-9  
RL: **CAT (Catalyst use)**; USES (Uses)  
(preparation of tri- and tetrasubstituted furans and pyrroles from **ruthenium-** and platinum- catalyzed propargylic alcs. and ketones)  
IT 62-53-3, Aniline, reactions 67-64-1, Acetone, reactions 78-93-3, Butanone, reactions 96-22-0, 3-Pentanone 106-47-8, 4-Chloroaniline, reactions 106-49-0, 4-Methylaniline, reactions 108-94-1, Cyclohexanone, reactions 120-92-3, Cyclopentanone 502-42-1, Cycloheptanone 3798-61-6 3857-25-8, 2-Hydroxymethyl-5-methylfuran **4187-87-5** 4187-88-6 7342-07-6 15100-93-3 19115-30-1 29805-11-6 83494-26-2 339987-26-7  
RL: RCT (Reactant); RACT (Reactant or reagent)



(preparation of tri- and tetrasubstituted furans and pyrroles from ruthenium- and platinum- catalyzed propargylic alcs. and ketones)

IT 13712-55-5P 19842-57-0P 25234-74-6P 57044-53-8P 88928-40-9P  
94964-57-5P 100909-93-1P 595598-35-9P 595598-36-0P  
595598-37-1P 595598-38-2P 595598-39-3P 595598-40-6P 595598-41-7P  
595598-42-8P 595598-43-9P 595598-44-0P 595598-45-1P 595598-46-2P  
595598-47-3P 595598-48-4P 595598-49-5P 595598-50-8P 595598-51-9P  
595598-52-0P

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(preparation of tri- and tetrasubstituted furans and pyrroles from ruthenium- and platinum- catalyzed propargylic alcs. and ketones)

RE.CNT 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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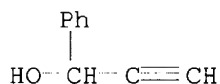
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IT 4187-87-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of tri- and tetrasubstituted furans and pyrroles from  
ruthenium- and platinum- catalyzed propargylic alcs. and ketones)

RN 4187-87-5 HCAPLUS

CN Benzenemethanol,  $\alpha$ -ethynyl- (9CI) (CA INDEX NAME)

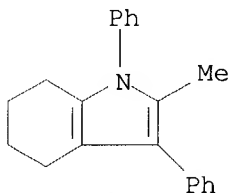


IT 94964-57-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of tri- and tetrasubstituted furans and pyrroles from  
ruthenium- and platinum- catalyzed propargylic alcs. and ketones)

RN 94964-57-5 HCAPLUS

CN 1H-Indole, 4,5,6,7-tetrahydro-2-methyl-1,3-diphenyl- (9CI) (CA INDEX NAME)



L36 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:696820 HCAPLUS

DN 137:384693

ED Entered STN: 15 Sep 2002

TI Ruthenium-Catalyzed Propargylation of Aromatic Compounds with Propargylic Alcohols

AU Nishibayashi, Yoshiaki; Yoshikawa, Masato; Inada, Youichi; Hidai, Masanobu; Uemura, Sakae

CS Department of Energy and Hydrocarbon Chemistry, Kyoto University, Kyoto, 606-8501, Japan

SO Journal of the American Chemical Society (2002), 124(40), 11846-11847  
CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society  
DT Journal  
LA English  
CC 27-1 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 25  
AB A novel ruthenium-catalyzed propargylation of aromatic compds. with propargylic alcs. has been found to afford the corresponding propargylated aromatic products in good yields with complete regioselectivity. The catalytic reaction is potentially useful in organic synthesis because the selective propargylation of aromatic compds. with an aromatic C-H bond cleavage is generally difficult.  
ST ruthenium complex propargylation arom heteroarom propargylic alc; regioselective propargylation arom heteroarom ruthenium complex  
IT Heterocyclic compounds  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(aromatic; ruthenium complex-catalyzed propargylation of aromatic and heteroarom. compds. with propargylic alcs.)  
IT Aromatic compounds  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(heterocyclic; ruthenium complex-catalyzed propargylation of aromatic and heteroarom. compds. with propargylic alcs.)  
IT Alcohols, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(propargyl; ruthenium complex-catalyzed propargylation of aromatic and heteroarom. compds. with propargylic alcs.)  
IT **Alkynylation**  
**Alkynylation catalysts**  
(propargylation; ruthenium complex-catalyzed propargylation of aromatic and heteroarom. compds. with propargylic alcs.)  
IT Aromatic compounds  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(ruthenium complex-catalyzed propargylation of aromatic and heteroarom. compds. with propargylic alcs.)  
IT 119970-52-4 191013-72-6 216064-22-1 340154-55-4  
RL: **CAT (Catalyst use)**; USES (Uses)  
(**ruthenium** complex-catalyzed propargylation of aromatic and heteroarom. compds. with propargylic alcs.)  
IT 216064-20-9  
RL: **CAT (Catalyst use)**; RCT (Reactant); RACT (Reactant or reagent); USES (Uses)  
(**ruthenium** complex-catalyzed propargylation of aromatic and heteroarom. compds. with propargylic alcs.)  
IT 91-66-7, N,N-Diethylaniline 96-54-8, 1-Methylpyrrole 109-97-7, Pyrrole 110-00-9, Furan 120-72-9, Indole, reactions 121-69-7, N,N-Dimethylaniline, reactions 122-39-4, N-Phenyldaniline, reactions 275-51-4, Azulene 496-15-1, Indoline 534-22-5, 2-Methylfuran 552-82-9, N-Methyl-N-phenylaniline 554-14-3, 2-Methylthiophene 621-23-8, 1,3,5-Trimethoxybenzene 635-90-5 824-21-5, 1-Methylindoline 1791-23-7 3208-16-0, 2-Ethylfuran 3798-61-6 **4187-87-5**,  $\alpha$ -Ethynylbenzyl alcohol 4187-88-6 7342-07-6 15100-93-3 18430-85-8, Pyrrole-d5 25414-22-6, 2-Methoxyfuran 29805-11-6 79257-61-7, 3',5'-Dimethoxyacetanilide 83494-26-2 100121-36-6 339987-26-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(ruthenium complex-catalyzed propargylation of aromatic and heteroarom. compds. with propargylic alcs.)  
IT 475625-31-1P 475625-32-2P 475625-33-3P 475625-34-4P 475625-35-5P  
475625-36-6P 475625-37-7P 475625-38-8P 475625-39-9P 475625-40-2P  
475625-41-3P 475625-42-4P 475625-43-5P 475625-44-6P 475625-45-7P

475625-46-8P 475625-47-9P 475625-48-0P 475625-49-1P 475625-50-4P  
475625-51-5P 475625-52-6P 475625-53-7P **475625-54-8P**  
475625-55-9P 475625-56-0P **475625-57-1P** 475625-58-2P  
475625-59-3P 475625-60-6P 475625-61-7P 475625-62-8P 475625-63-9P  
475625-64-0P 475625-65-1P **475625-66-2P** 475625-67-3P

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(ruthenium complex-catalyzed propargylation of aromatic and heteroarom.  
compds. with propargylic alcs.)

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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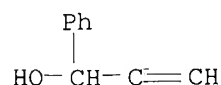
IT **4187-87-5,  $\alpha$ -Ethynylbenzyl alcohol**

RL: RCT (Reactant); RACT (Reactant or reagent)

(ruthenium complex-catalyzed propargylation of aromatic and heteroarom.  
compds. with propargylic alcs.)

RN 4187-87-5 HCAPLUS

CN Benzenemethanol,  $\alpha$ -ethynyl- (9CI) (CA INDEX NAME)



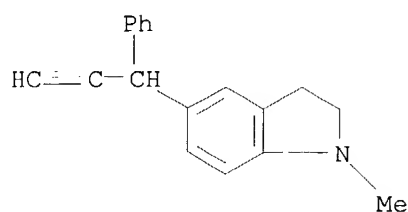
IT **475625-54-8P 475625-57-1P 475625-66-2P**

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(ruthenium complex-catalyzed propargylation of aromatic and heteroarom.  
compds. with propargylic alcs.)

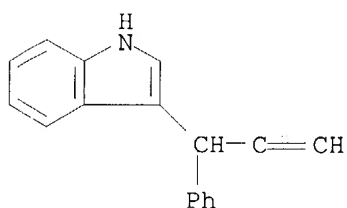
RN 475625-54-8 HCAPLUS

CN 1H-Indole, 2,3-dihydro-1-methyl-5-(1-phenyl-2-propynyl)- (9CI) (CA INDEX NAME)



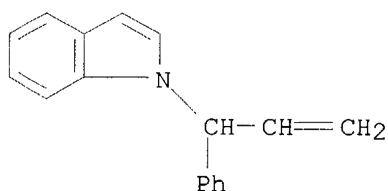
RN 475625-57-1 HCAPLUS

CN 1H-Indole, 3-(1-phenyl-2-propynyl)- (9CI) (CA INDEX NAME)



RN 475625-66-2 HCAPLUS

CN 1H-Indole, 1-(1-phenyl-2-propenyl)- (9CI) (CA INDEX NAME)



L36 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:112680 HCAPLUS

DN 136:294702

ED Entered STN: 12 Feb 2002

TI Regioselective Synthesis of Indoles via Reductive Annulation of Nitrosoaromatics with **Alkynes**

AU Penoni, Andrea; Volkmann, Jerome; Nicholas, Kenneth M.

CS Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK, 73019, USA

SO Organic Letters (2002), 4(5), 699-701

CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

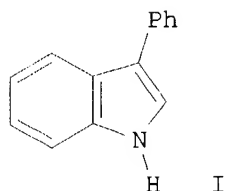
DT Journal

LA English

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

OS CASREACT 136:294702

GI



- AB Indoles, e.g., I, are produced regioselectively and in moderate yields by two new processes: (a) from the [Cp\*Ru(CO)<sub>2</sub>]<sub>2</sub>-catalyzed reaction of nitrosoaroms. (ArNO) with **alkynes** under carbon monoxide and (b) in a two-step sequence involving the (uncatalyzed) reaction of ArNO with **alkynes**, followed by reduction of the intermediate adduct.
- ST nitrosoarom **alkyne** regioselective reductive annulation; indole prepn; regioselective reductive annulation catalyst ruthenium; **alkyne** nitrosoarom regioselective cycloaddn hydrogenation
- IT Aromatic compounds  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(nitroso; regioselective preparation of indoles via cycloaddn. of nitrosoaroms. with **alkynes** and subsequent hydrogenation of intermediate N-hydroxy indoles)
- IT Cycloaddition reaction  
(regioselective)
- IT Cycloaddition reaction catalysts  
(regioselective preparation of indoles via cycloaddn. of nitrosoaroms. with **alkynes** and subsequent hydrogenation of intermediate N-hydroxy indoles)
- IT **Alkynes**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(regioselective preparation of indoles via cycloaddn. of nitrosoaroms. with **alkynes** and subsequent hydrogenation of intermediate N-hydroxy indoles)
- IT 611-23-4 623-47-2 629-05-0, 1-Octyne 762-21-0 932-98-9 3623-23-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(regioselective preparation of indoles via cycloaddn. of nitrosoaroms. with **alkynes** and subsequent hydrogenation of intermediate N-hydroxy indoles)
- IT **56830-62-7P 409059-35-4P 409059-36-5P 409059-37-6P 409059-38-7P**  
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**; RACT (Reactant or reagent)  
(regioselective preparation of indoles via cycloaddn. of nitrosoaroms. with **alkynes** and subsequent hydrogenation of intermediate N-hydroxy indoles)
- IT **776-41-0P 22072-89-5P 52604-06-5P 54470-19-8P 56366-16-6P 128942-88-1P**  
RL: **SPN (Synthetic preparation); PREP (Preparation)**  
(regioselective preparation of indoles via cycloaddn. of nitrosoaroms. with **alkynes** and subsequent hydrogenation of intermediate N-hydroxy indoles)
- IT 62-53-3P, Aniline, preparation 103-33-3P, Azobenzene 495-48-7P, Azoxybenzene  
RL: **BYP (Byproduct); PREP (Preparation)**  
(regioselective preparation of indoles via ruthenium catalyzed reductive annulation of nitrosoaroms. with **alkynes**)
- IT 70669-56-6

RL: **CAT (Catalyst use); USES (Uses)**

(regioselective preparation of indoles via **ruthenium** catalyzed reductive annulation of nitrosoaroms. with **alkynes**)

IT 120-22-9 536-74-3, Phenylacetylene 586-96-9, Nitrosobenzene  
673-32-5, 1-Phenyl-1-propyne 2216-94-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(regioselective preparation of indoles via ruthenium catalyzed reductive annulation of nitrosoaroms. with **alkynes**)

IT 1504-16-1P, 3-Phenylindole 4757-69-1P  
37129-23-0P 409059-34-3P

RL: **SPN (Synthetic preparation); PREP (Preparation)**

(regioselective preparation of indoles via ruthenium catalyzed reductive annulation of nitrosoaroms. with **alkynes**)

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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HCAPLUS

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IT 56830-62-7P 409059-35-4P 409059-36-5P

409059-37-6P 409059-38-7P

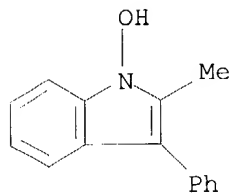
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP**

**(Preparation); RACT (Reactant or reagent)**

(regioselective preparation of indoles via cycloaddn. of nitrosoaroms. with **alkynes** and subsequent hydrogenation of intermediate N-hydroxy indoles)

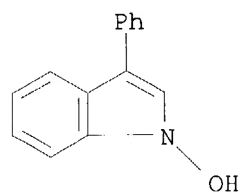
RN 56830-62-7 HCAPLUS

CN 1H-Indole, 1-hydroxy-2-methyl-3-phenyl- (9CI) (CA INDEX NAME)



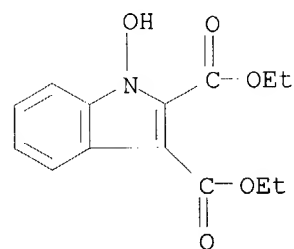
RN 409059-35-4 HCAPLUS

CN 1H-Indole, 1-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)



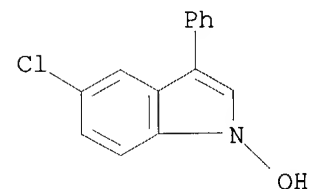
RN 409059-36-5 HCAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, 1-hydroxy-, diethyl ester (9CI) (CA INDEX NAME)



RN 409059-37-6 HCAPLUS

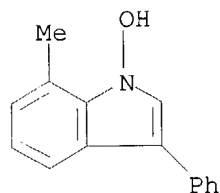
CN 1H-Indole, 5-chloro-1-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)



RN 409059-38-7 HCAPLUS

CN 1H-Indole, 1-hydroxy-7-methyl-3-phenyl- (9CI) (CA INDEX NAME)





IT 776-41-0P 22072-89-5P 52604-06-5P

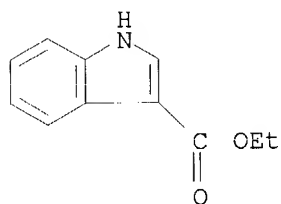
54470-19-8P 56366-16-6P 128942-88-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(regioselective preparation of indoles via cycloaddn. of nitrosoaroms. with alkynes and subsequent hydrogenation of intermediate N-hydroxy indoles)

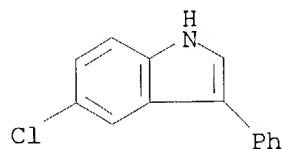
RN 776-41-0 HCAPLUS

CN 1H-Indole-3-carboxylic acid, ethyl ester (9CI) (CA INDEX NAME)



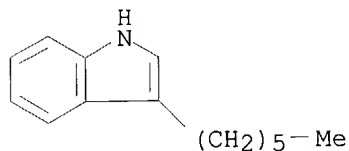
RN 22072-89-5 HCAPLUS

CN 1H-Indole, 5-chloro-3-phenyl- (9CI) (CA INDEX NAME)



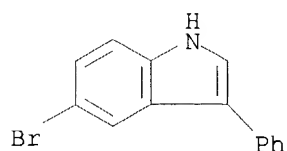
RN 52604-06-5 HCAPLUS

CN 1H-Indole, 3-hexyl- (9CI) (CA INDEX NAME)



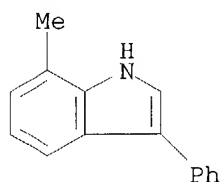
RN 54470-19-8 HCAPLUS

CN 1H-Indole, 5-bromo-3-phenyl- (9CI) (CA INDEX NAME)



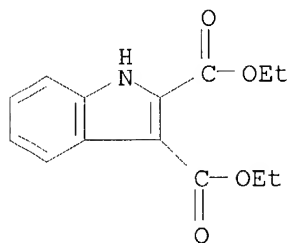
RN 56366-16-6 HCAPLUS

CN 1H-Indole, 7-methyl-3-phenyl- (9CI) (CA INDEX NAME)



RN 128942-88-1 HCAPLUS

CN 1H-Indole-2,3-dicarboxylic acid, diethyl ester (9CI) (CA INDEX NAME)



IT 1504-16-1P, 3-Phenylindole 4757-69-1P

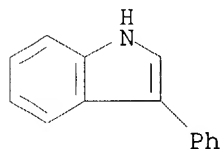
37129-23-0P 409059-34-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(regioselective preparation of indoles via ruthenium catalyzed reductive annulation of nitrosoaroms. with **alkynes**)

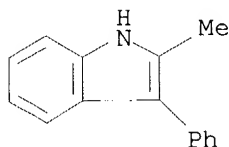
RN 1504-16-1 HCAPLUS

CN 1H-Indole, 3-phenyl- (9CI) (CA INDEX NAME)



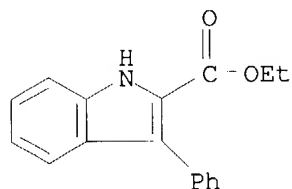
RN 4757-69-1 HCAPLUS

CN 1H-Indole, 2-methyl-3-phenyl- (9CI) (CA INDEX NAME)



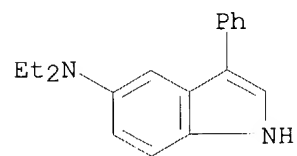
RN 37129-23-0 HCAPLUS

CN 1H-Indole-2-carboxylic acid, 3-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 409059-34-3 HCAPLUS

CN 1H-Indol-5-amine, N,N-diethyl-3-phenyl- (9CI) (CA INDEX NAME)



L36 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:177653 HCAPLUS

DN 135:46061

ED Entered STN: 15 Mar 2001

TI Ruthenium-catalyzed intramolecular hydroamination of aminoalkynes

AU Kondo, T.; Okada, T.; Suzuki, T.; Mitsudo, T.-a.

CS Department of Energy and Hydrocarbon Chemistry, Graduate School of Engineering, Kyoto University, Kyoto, Sakyo-ku, 606-8501, Japan

SO Journal of Organometallic Chemistry (2001), 622(1-2), 149-154

CODEN: JORCAI; ISSN: 0022-328X

PB Elsevier Science S.A.

DT Journal

LA English

CC 27-10 (Heterocyclic Compounds (One Hetero Atom))

OS CASREACT 135:46061

AB Low-valent ruthenium complexes with a  $\pi$ -acidic ligand, such as  $\text{Ru}(\eta^6\text{-cot})(\text{dmfm})_2$  [ $\text{cot}$ =1,3,5-cyclooctatriene,  $\text{dmfm}$ =dimethyl fumarate] and  $\text{Ru}_3(\text{CO})_{12}$ , showed high catalytic activity for the intramolecular hydroamination of aminoalkynes. The reaction is highly regioselective, in which a nitrogen atom is selectively attached to an internal carbon of **alkynes** to give five-, six-, and seven-membered nitrogen heterocycles as well as indoles in good to high yields.

ST regiochem **alkynyl** amine hydroamination ruthenium; cyclization aminoalkyne; pyrrole dihydro prep; cyclic amine prep; pyridine tetrahydro prep; indole prep; azepine tetrahydro prep

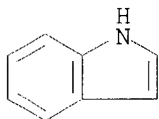
- IT Amines, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(alkynyl; ruthenium-catalyzed intramol. hydroamination of aminoalkynes)
- IT Amines, preparation  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(cyclic; ruthenium-catalyzed intramol. hydroamination of aminoalkynes)
- IT Cyclization  
Cyclization catalysts  
(preparation of cyclic amines by ruthenium-catalyzed intramol. hydroamination of aminoalkynes)
- IT Amination  
Amination catalysts  
(reductive; ruthenium-catalyzed intramol. hydroamination of aminoalkynes)
- IT 14741-36-7 15243-33-1, Triruthenium dodecacarbonyl [Ru<sub>3</sub>(CO)<sub>12</sub>]  
15529-49-4, Dichlorotris(triphenylphosphine)ruthenium  
19529-00-1, Dihydrotetrakis(triphenylphosphine)ruthenium  
31781-74-5 37366-09-9 42516-72-3 74577-86-9 92390-26-6  
131659-92-2 223249-01-2  
RL: CAT (Catalyst use); USES (Uses)  
(preparation of cyclic amines by ruthenium-catalyzed intramol. hydroamination of aminoalkynes)
- IT 15252-44-5, 4-Pentyn-1-amine 52670-38-9, 2-Ethynylaniline 120788-31-0,  
4-Hexyn-1-amine 127808-49-5, 5-Phenyl-4-pentyn-1-amine 135469-76-0,  
6-phenyl-5-hexyn-1-amine 154188-72-4, 7-phenyl-6-heptyn-1-amine  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of cyclic amines by ruthenium-catalyzed intramol. hydroamination of aminoalkynes)
- IT 344738-98-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of cyclic amines by ruthenium-catalyzed intramol. hydroamination of aminoalkynes)
- IT 120-72-9P, 1H-Indole, preparation 872-32-2P,  
3,4-Dihydro-5-methyl-2H-pyrrole 1192-29-6P 3338-08-7P 68840-81-3P  
69311-30-4P 95018-41-0P 344738-99-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of cyclic amines by ruthenium-catalyzed intramol. hydroamination of aminoalkynes)

RE.CNT 94 THERE ARE 94 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE

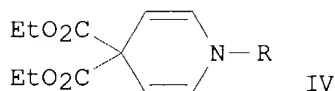
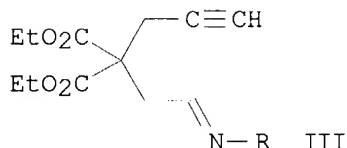
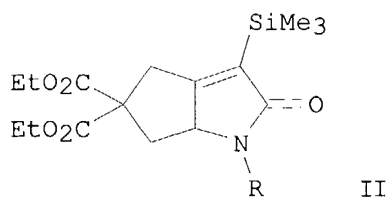
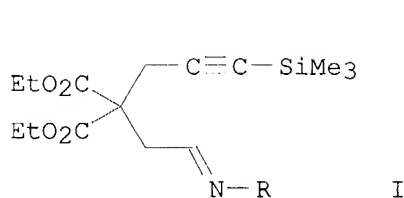
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IT 120-72-9P, 1H-Indole, preparation  
RL: **SPN (Synthetic preparation); PREP (Preparation)**  
(preparation of cyclic amines by ruthenium-catalyzed intramol.  
hydroamination of aminoalkynes)  
RN 120-72-9 HCAPLUS  
CN 1H-Indole (9CI) (CA INDEX NAME)



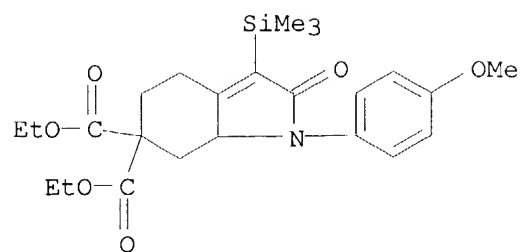
L36 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 1999:405925 HCAPLUS  
DN 131:170241  
ED Entered STN: 01 Jul 1999  
TI Ru<sub>3</sub>(CO)<sub>12</sub>-catalyzed reaction of yne-imines with carbon monoxide leading to bicyclic  $\alpha,\beta$ -unsaturated lactams  
AU Chatani, Naoto; Morimoto, Tsumoru; Kamitani, Akihito; Fukumoto, Yoshiya; Murai, Shinji  
CS Faculty of Engineering, Department of Applied Chemistry, Osaka University, Suita, Osaka, Japan  
SO Journal of Organometallic Chemistry (1999), 579(1-2), 177-181  
CODEN: JORCAI; ISSN: 0022-328X  
PB Elsevier Science S.A.  
DT Journal  
LA English  
CC 27-10 (Heterocyclic Compounds (One Hetero Atom))  
OS CASREACT 131:170241  
GI



- AB The cyclocarbonylation of 1,6- and 1,7-yne-imines, e.g., I (R = 4-MeOC6H4), leading to bicyclic  $\alpha,\beta$ -unsatd. lactams, e.g., II (R = 4-MeOC6H4), can be achieved in the presence of a catalytic amount of Ru<sub>3</sub>(CO)<sub>12</sub>. The reaction, a [2+2+1] cycloaddn., incorporates the acetylene  $\pi$ -bond, the imine  $\pi$ -bond, and the carbon atom of CO. The presence of substituents, such as alkyl, aryl, and silyl on the acetylenic terminal carbon is essential for yne-imines to undergo cyclocarbonylation to give bicyclic  $\alpha,\beta$ -unsatd. lactams. An yne-imine having no substituents on the acetylenic terminal carbon, III (R = 4-MeOC6H4), does not give the corresponding lactam, but rather a dihydropyridine derivative, IV (R = 4-MeOC6H4), without incorporating CO.
- ST cyclocarbonylation **alkyne** imine ruthenium; carbonylation cyclo **alkyne** imine ruthenium; lactam bicyclic unsatd prepn
- IT Carbonylation  
Carbonylation catalysts  
(cyclo-; ruthenium-catalyzed cyclocarbonylation of yne-imines to bicyclic unsatd. lactams)
- IT Imines  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(yne; ruthenium-catalyzed cyclocarbonylation of yne-imines to bicyclic unsatd. lactams)
- IT Lactams  
RL: SPN (Synthetic preparation); PREP (Preparation)  
( $\alpha,\beta$ -unsatd.; ruthenium-catalyzed cyclocarbonylation of yne-imines to bicyclic unsatd. lactams)
- IT 238746-21-9P  
RL: PNU (Preparation, unclassified); PREP (Preparation)  
(failed ruthenium-catalyzed cyclocarbonylation of yne-imines with a tert-Bu N protecting group)
- IT 238746-02-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(failed ruthenium-catalyzed cyclocarbonylation of yne-imines without a terminal **alkyne** substituent and formation of a dihydropyridine derivative)
- IT 238746-04-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(failed ruthenium-catalyzed cyclocarbonylation of yne-imines without a terminal **alkyne** substituent and formation of a dihydropyridine derivative)

- IT 15243-33-1, Triruthenium dodecacarbonyl  
 RL: **CAT (Catalyst use); USES (Uses)**  
 (ruthenium-catalyzed cyclocarbonylation of yne-imines to bicyclic unsatd. lactams)
- IT 238745-88-5 238745-91-0 238745-94-3 238745-96-5 238745-99-8  
 238746-06-0 238746-08-2 238746-10-6 238746-12-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (ruthenium-catalyzed cyclocarbonylation of yne-imines to bicyclic unsatd. lactams)
- IT 238745-90-9P 238745-92-1P 238745-95-4P 238745-98-7P  
**238746-00-4P** 238746-14-0P 238746-16-2P 238746-17-3P  
 238746-19-5P  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (ruthenium-catalyzed cyclocarbonylation of yne-imines to bicyclic unsatd. lactams)
- RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
- RE
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- IT **238746-00-4P**  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (ruthenium-catalyzed cyclocarbonylation of yne-imines to bicyclic unsatd. lactams)
- RN 238746-00-4 HCAPLUS
- CN 6H-Indole-6,6-dicarboxylic acid, 1,2,4,5,7,7a-hexahydro-1-(4-methoxyphenyl)-2-oxo-3-(trimethylsilyl)-, diethyl ester (9CI) (CA INDEX NAME)





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